

### Updates to the SMART Algorithm

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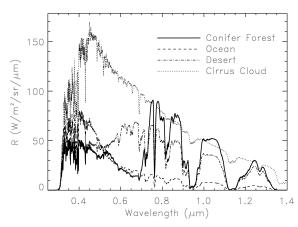
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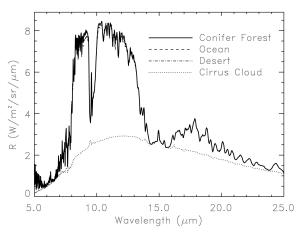


# Radiative Transfer in Scattering/Absorbing/Emitting Atmospheres

- Efficient, accurate methods for simulating the absorption, emission, and scattering of solar and thermal radiation are essential for:
  - Analysis of remote sensing observations
  - Radiative heating and cooling rate calculations for climate models
- These problems are intrinsically challenging when fluxes or radiances are needed over broad spectral regions because
  - Gas absorption cross sections change rapidly with wavelength
  - Methods for estimating radiances and fluxes in the presence of multiple scattering must be applied to spectral regions that are sufficiently narrow that the optical properties are essentially constant (monochromatic)







**Emitted Thermal Radiation** 



### Exact Methods for Solving Radiative Transfer Problems in Wide Spectral Regions

- The most accurate solutions to the equation of transfer in scattering, absorbing, emitting atmospheres can be obtained from "full-physics" methods that
  - Employ a spectral grid that is fine enough to resolve the spectral structure of all (gas, aerosol, surface) optical properties, and their variations along the optical path
  - Perform a (vector or scalar) multi-stream, multiple scattering calculation at each spectral grind point
- The primary problem with this approach is its computational expense, especially for broad-band (bolometric) calculations
  - 10<sup>6</sup> to 10<sup>7</sup> spectral grid points are needed to fully resolve the spectral structure throughout the solar and thermal spectral range
  - 4 to 8 vertical grid points are needed per scale height to accurately resolve the pressure and temperature dependent changes in the gas absorption cross-sections and the vertical structure of clouds and aerosols
  - 8 to 256 "streams" are needed to resolve the angle dependence of the radiation field



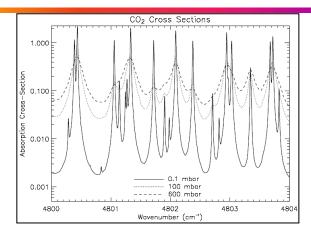
### Spectral Mapping Methods for High Resolution Spectra: SMART

- Spectral Mapping exploits the fact that many spectral regions have "similar" optical properties at all points along the optical path
  - Similar regions can be "binned" and radiances can be calculated for each bin
  - A spectral "map" is created so that the "binned" radiances can be mapped back to the original, high-resolution spectral grid.
- The basic procedure includes the following steps:
  - Define a spectral grid that completely resolves the wavelength-dependent optical properties of the surface and all gases, clouds, and aerosols that contribute to the radiation field throughout the atmospheric column;
  - Identify spectral grid points that have similar optical properties along the entire surface/atmosphere optical path;
  - Map these grid points into a smaller number of quasi-monochromatic bins;
  - Use a multi-stream multiple scattering algorithm calculate the angledependent radiances for each bin; and
  - Map these radiances back to their original spectral grid points to create a high-resolution spectrum.

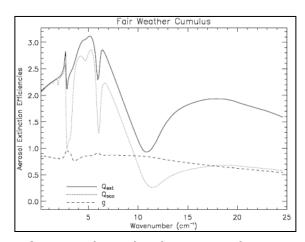


#### Components of the Spectral Grid

- A very fine grid is needed to resolve narrow vibration-rotation absorption lines:
  - Our line-by-line model (LBLABC) uses a nonuniform grid, with finer resolution near line centers and courser spacing elsewhere.
  - Much coarser grids are adequate to resolve:
    - Gas electronic transitions in the visible and UV
    - Pressure-induced absorption by gases at infrared wavelengths
  - A course grid is also adequate to resolve
    - The wavelength dependent single scattering optical properties of clouds and aerosols
    - The wavelength dependent surface reflectance.
- To address the needs, SMART uses a "lowest common denominator" spectral grid
  - preserves all of the spectral structure included in the input files.
  - Minimizes the number of spectral grid points



Gas Absorption coefficients vary rapidly with wavelength.



Aerosol optical properties vary much more slowly.



### Spectral Binning in SMART

- Each Spectral Bin is defined by a mean value and a range of acceptable values at each atmospheric level and at the surface:
  - Mean Values:  $x_b = [\delta \tau_b(z), \omega_b(z), g_b(z), a_b]$
  - Range:  $\Delta \delta \tau_b(z)$ ,  $\Delta \omega_b(z)$ ,  $\Delta g_b(z)$ ,  $\Delta a_b$ 
    - Set by the user at run time
- A monochromatic grid point is included in a bin if it satisfies the following criteria at all levels:

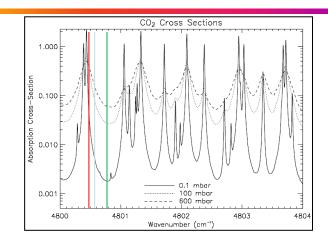
Differential Optical depth:  $\delta \tau(z) = \delta \tau_b(z) \pm \Delta \delta \tau_b(z)$ 

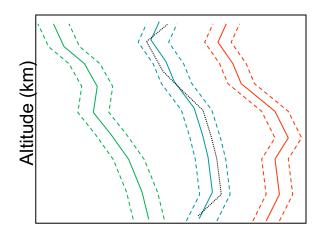
Single Scattering Albedo:  $\omega(z) = \omega_b(z) \Delta \omega_b(z)$ 

Asymmetry Parameter:  $g(z) = g_b(z) \pm \Delta g_b(z)$ 

Surface Albedo  $\triangle a = a_b \pm \triangle a_b$ 

- If the sounding fits in a bin, the bin number is recorded on the "Spectral Map"
- If a sounding does not fit in an existing bin, a new bin is defined and initialized with by its optical properties





Cartoon showing differential optical depths,  $\delta \tau(z)$  for 3 bins (blue, green, red).



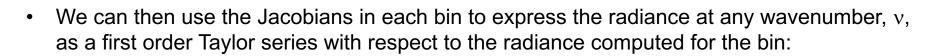
#### Improving the Accuracy of the Spectral Mapping

The spectral mapping scheme in current version of SMART has been modified to improve the accuracy and efficiency:

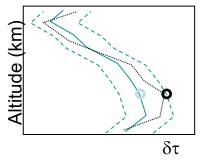
- Radiances are assumed to vary linearly with optical property variations within each bin
- SMART finds radiances for:
  - The mean optical properties of each bin
  - Perturbed values:  $\delta x_b(z) + \delta x_b'(z)$
- Radiance fields for mean and perturbed cases are used to estimate the rate of change of the radiance with layer optical properties: the radiance Jacobians:

$$J = \partial r_i / \partial x_i$$

These quantities specify the rate of change of the radiances,  $\mathbf{r}$ , at any level, i, due to changes in optical property,  $\mathbf{x} = \delta \tau(\mathbf{z})$ ,  $\omega(\mathbf{z})$ ,  $g(\mathbf{z})$ , a, at level,  $\mathbf{i}$ .



$$r(v) = r_b + \sum \partial r_{bi} / \partial \tau_{bj} (\delta \tau_j(v) - \delta \tau_{bj}) + \partial r_{bi} / \partial \omega_{bj} (\omega_j(v) - \omega_{bj}) + \partial r_{bi} / \partial g_{bj} (g_j(v) - g_{bj})$$

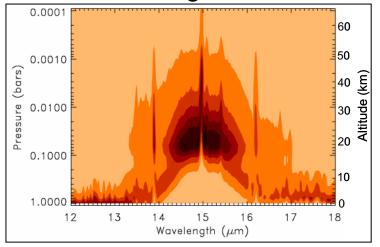




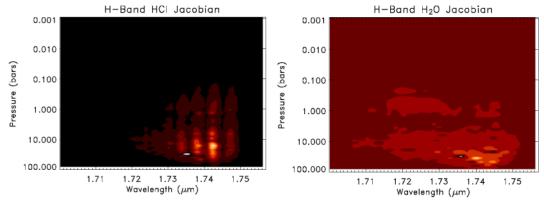
### Other Benefits: Jacobians for Remote Sensing Algorithms

 The accuracy and efficiency of the linearized method for mapping the binned values back to the original spectral grid also provides and efficient method for generating Jacobians for use in remote sensing

retrieval algorithms



Temperature Jacobians (weighting functions) are shown for the 15- $\mu$ m CO<sub>2</sub> band in the Earth's atmosphere .



Jacobians (weighting functions) for HCl (left) and  $H_2O$  are shown for the 1.74- $\mu$ m atmospheric window on the night side of Venus. Jacobians like these will be used to analyze Venus Express observations of the Venus atmosphere to assess the abundances of trace gases below the planet-encircling sulfuric acid cloud deck.



#### **Updating SMART**

#### We are in the process of updating SMART to

- Convert from FORTRAN 77 to FORTRAN 9X to improve maintainability
- Change the core radiative transfer model from DISORT to the Linearized Discrete Ordinate Radiative Transfer (LIDORT) algorithm
- Exploit additional opportunities to improve the performance of the SMART-LIDORT model.

#### Over the remainder of calendar year 2019, we plan to:

 Create a no-binning path within SMART that uses LIDORT to generate high spectral resolution radiances, fluxes, and their Jacobians directly from the wavelength-dependent optical properties without binning and remapping. This will replace the capabilities of the obsolete DART model. This path will be too slow for routine calculations, but will provide a critical tool for testing the accuracy of SMART's binned/remapped results;



## Simplify and Speed Up Solar/Stellar Radiance and Flux Calculations

- Replace the 2-D adding method with direct use of LIDORT's analytic
  Jacobians for mapping solar/stellar radiances and fluxes from each
  spectral bin back to the high resolution spectrum.
  - This effort should fully exploit the analytic Jacobians produced by LIDORT to increase the speed and accuracy of these calculations
  - We will also explore the option of separating the single scattering and multiple scattering in each calculation, so that the multiple scattering results are binned and remapped, and the single scattering results are generated directly at each spectral point, without binning or remapping.
  - This is a significant structural change in SMART and is likely to dominate this phase of the development, but should substantially increase the speed, accuracy, and reliability of the model;
- Collaborate with the VPL team to develop an approach for integrating the Transit branch back into the SMART code;



#### Complete the Scalar Model

- Complete the implementation of LIDORT in the scalar version of the SMART model and produce a stable version that can be fully tested and validated by the VPL team;
  - Complete implementation of radiance and flux Jacobian output.
  - Complete implementation and testing of methods to handle optical property input files that do not span the entire spectral range requested.
  - Complete the updates to replace internal I/O (scratch files) with buffers to facilitate use on computer clusters.
  - Complete effort to identify and implement OpenMP parallel constructs.
  - Profile the performance to improve performance on computer clusters and make reasonable performance modifications based on this profiling.
  - Update the error handling within SMART so that errors and warnings generated by SMART are sent to a SMART error file and errors produced by LIDORT are sent to a separate LIDORT error file, and a comment is added the SMART error file pointing the user to the LIDOR error file.
  - Extend the testing suite and continue testing SMART-LIDORT for different BRDFs and combinations of gas and aerosol absorption and scattering.



#### Next Steps - Transit and Polarization

- Continue the development of a streamlined F90 version of VLIDORT in a vector version of the SMART algorithm:
  - Streamline the standard version of VLIDORT for use in SMART (VLIDORT features to be retained would be TBD).
  - Create a separate set of the SMART-VLIDORT interface subroutines based on the SMART-LIDORT interfaces in the scalar version of SMART.
  - Make mods to SMART's input subroutines to accommodate the additional needed vector inputs for VLIDORT.
  - Run some training cases for the NSTOKES=1 scenario and insure the vector version of SMART agrees with the scalar version for this setup and then repeat the cases for a fuller NSTOKES=3 scenario.
  - Modify the scalar user guide as appropriate to create a user guide for the vector version of SMART.
  - Continue to provide insight into specific variables and algorithmic approaches for optimizing the use of LIDORT & VLIDORT in the SMART algorithm and provide advice and recommendations to VPL as needed.



# Other Ongoing Efforts – Modifications to the SMART I/O

- While the internal changes described above will dominate the development activities over the next few months, we are also initiating series of changes in the I/O interface to enhance portability of input files and output products and facilitate interactions with GCMs and to:
  - An option will be added to read in the gas, aerosol, and surface optical property files in netCDF and HDF5 formats
  - An option to write output flux, radiance and Jacobian files as netCDF and HDF files
  - We will also explore options for reading in atmospheric structure, gas mixing ratios and cloud distributions from netCDF and HDF5 files
- The SMART "classic" interface will be preserved to the extent possible to facilitate the use of legacy run scripts and wrapper files, but may require a few new flags
- Let us know if you want to enable SMART-LIDORT to read or write to a specific type of netCDF of HDF5 file